Velocity correlation of a lipid in the lipid-bilayer membrane at the equilibrium

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我々は脂質二重膜上の脂質分子の自己拡散を考える。膜は揺らいでおり、曲げ弾性をもつ圧縮性の2次元流体で、非圧縮 Stokes 流体中に挟まれていると考える。揺動散逸定理から速度場の相関を求め、モード結合理論を用いると、脂質分子の速度相関の表式は速度場を用いて表される。こうして典型的なパラメータに対して得られた速度相関の表式を数値積分した結果によれば、相関関数の時間依存性は時間 t が大きくなるにつれて t^{-1} から $t^{-3/2}$ に遷移することがわかった。

The velocity correlation function (VCF) of a tracer particle decays away as $t^{-d/2}$ as the time t tends to the infinity in a d -dimensional equilibrium fluid[1]. The Brownian particle — a larger impurity particle — also has this long time tail[2]. A biomembrane is a two-dimensional (2D) fluid surrounded with three-dimensional fluids. A membrane protein can be regarded as a Brownian particle[3]. Sera & Rubi[4] showed theoretically that both t^{-1} and $t^{-3/2}$ appear in its velocity correlation[4]. This is reasonable, considering that the momentum on the membrane spread out into the outer fluids. Seki & Komura[5] obtained similar results in a more simple way by introducing a phenomenological momentum relaxation time τ which represents coupling strength between the membrane and the outer fluids. The VCF of the membrane protein was found to decay as $e^{-t/\tau}t^{-3/2}$ or $e^{-t/\tau}t^{-1}$ in the case of the strong- or the weak- coupling limits, respectively.

We study the VCF of the lipid molecule not a membrane protein. We assume that the lipid-bilayer membrane is a compressive 2D Newtonian fluid with the bending rigidity. It fluctuates about the equilibrium in the fluids on its both sides. Using unsteady Stokes approximation, we obtain the Eulerian VCF, $\langle \boldsymbol{v}(\boldsymbol{k},t)\cdot \boldsymbol{v}(\boldsymbol{k}',t')\rangle$, with the aid of the linear response theory[6]. Here, the angular brackets represent the equilibrium ensemble average, while $\boldsymbol{v}(\boldsymbol{k},t)$ denotes the Eulerian velocity field with $\boldsymbol{k}$ representing the wave number vector.

Writing $\boldsymbol{V}(t)$ for a lipid molecule velocity, apart from the fast decaying term, we have

$$\langle \boldsymbol{V}(t)\cdot \boldsymbol{V}(0)\rangle \propto D(t) \equiv \int_0^{k_U} d\boldsymbol{k} e^{-D_0 k^2 t}\langle \boldsymbol{v}(\boldsymbol{k},t)\cdot \boldsymbol{v}(\boldsymbol{k},0)\rangle \tag{1}$$

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in terms of the mode-coupling theory. Here, k_U is a upper cutoff wave number and D_0 is a 'bare' diffusion coefficient, which is independent of the hydrodynamics. We can evaluate its value in terms of the vacancy assisted diffusion[7].

Integrating right-hand side of (1) numerically by use of typical values, we obtain results shown as crosses in Fig.1. Two dotted lines with the slope of -1 and $-\frac{3}{2}$ are shown as guides. We can find that the VCF shifts from t^{-1} to $t^{-\frac{3}{2}}$ as t increases. We are now studying which factor gives the time around which the transition takes place.

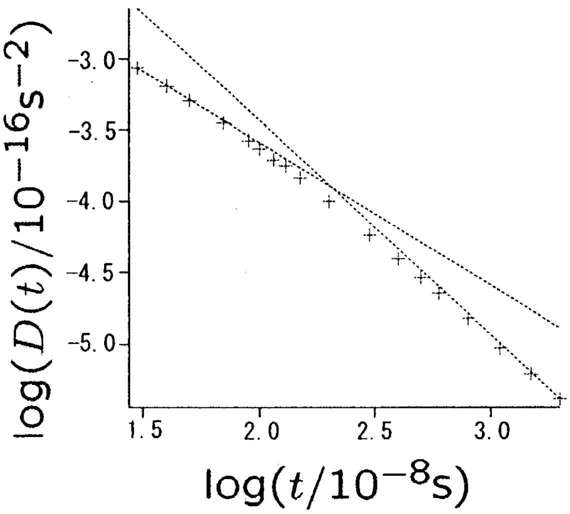

Figure 1: The behaviour of $D(t)$

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